

**SATELLITE-BASED STRATOSPHERIC AND TROPOSPHERIC MEASUREMENTS:
DETERMINATION OF GLOBAL OZONE AND OTHER TRACE SPECIES**

NASA Grant NAG5-10327

Final Report
For the period 1 January 2001 through 30 September 2002

Principal Investigator
Kelly Chance

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Introduction

This grant is an extension to our previous NASA Grant NAG5-3461, providing incremental funding to continue GOME and SCIAMACHY studies. This report summarizes research done under these grants through December 31, 2002. The research performed during this reporting period includes development and maintenance of scientific software for the GOME retrieval algorithms, consultation on operational software development for GOME, consultation and development for SCIAMACHY near-real-time (NRT) and off-line (OL) data products, and participation in initial SCIAMACHY validation studies. The Global Ozone Monitoring Experiment was successfully launched on the ERS-2 satellite on April 20, 1995, and remains working in normal fashion. SCIAMACHY was launched March 1, 2002 on the ESA Envisat satellite. Three GOME-2 instruments are now scheduled to fly on the Metop series of operational meteorological satellites (Eumetsat). K. Chance is a member of the reconstituted GOME Scientific Advisory Group, which will guide the GOME-2 program as well as the continuing ERS-2 GOME program.

GOME

GOME is a European Space Agency Program, with scientific participation from European countries and, in the U.S., the SAO and the NASA Goddard Space Flight Center. The GOME Science Advisory Group (GSAG) includes K. Chance of the SAO as a U.S. member and head of the Data and Algorithm Subcommittee, and R. Spurr of the SAO as a U.S. member and organizer and chair of the GOME/GOME Scientific Working Sessions. SAO GOME studies include the following items:

- Development of scientific code for implementation as GOME operational retrieval algorithms.
- Guiding the development of GOME Level 0-1 and 1-2 operational software through extensive collaboration with the German Aerospace Center (DLR). SAO compiled and installed in the DLR GOME data processor a new snow and ice coverage data set (originating from NASA as used in TOMS work). In addition, we developed a tessellation algorithm for the production of representative mixed-scene albedos for GOME footprints. This is especially valuable for pixels with ocean/ice interfaces, where incorrect albedo choices can severely affect O_3 column and profile retrieval accuracy.
- Cloud studies, including investigation of fitting schemes and analysis of uncertainties due to various error sources, including line parameters of O_2 . These resulted in production of the prototype operational algorithm for GOME cloud correction which has now been implemented in the Level 1 operational software.
- Collaboration on the development of DOAS operational procedures for GOME Level 1-2 processing to produce O_3 , NO_2 , and potentially other trace gas columns from GOME. This collaboration includes code development, measurement window selection, and a number of related issues. Development of direct of direct (*i.e.*, non-DOAS, or BOAS) fitting to improved the precision of trace gas measurements. Collaboration with DLR in development of an operational processor for BrO. Implementation of the SBUV, and its testing for a variety of simulated GOME measurements. Collaboration in development of the GOMEtran finite difference forward model.
- Development of a linearized discrete ordinate radiative transfer code (LIDORT) for retrieval and forward model studies in inhomogeneous scattering atmospheres [Spurr *et al.*, 2001]. In this work, the full multiple scatter backscatter intensity solution has been subject to an internal perturbation analysis, thus allowing the model to generate whole fields of weighting functions simultaneously. This is a vital requirement for non-linear iterative retrieval algorithms; the generic formalism of LIDORT enables it to be used in a

wide variety of remote sensing problems. Further developments include a model with the “pseudo-spherical” approximation wherein the direct beam attenuation is handled in a spherical atmosphere. The application of LIDORT to GOME and SCIAMACHY is direct and immediate. One of the most important uses will be for the performance enhancement of the ozone profile retrieval algorithm for both instruments. This goes a long way to the realization of operational O₃ profile retrieval algorithms. Work toward this goal has started in collaboration with DLR. LIDORT is also used in studies of tropospheric species from GOME, including HCHO and NO₂, to provide the scattering weights versus altitude which determine the relative source strength reflected in GOME measurements.

- Participation in GOME validation and scientific studies. Science studies include measurements of BrO, HCHO, NO₂, and height-resolved O₃.
- Radiative transfer studies related to wavelength calibration and spatial and spectral aliasing, including collaboration with the DLR to implement an alternative wavelength calibration method based on cross-correlation with a Fraunhofer reference spectrum (see Caspar and Chance, 1997) and correction for most of the effects of spectral undersampling by GOME [Chance, 1998; Slijkhuis *et al.*, 1999]. Our undersampling correction technique has now been adopted by the University of Bremen IFE and Belgian IASB groups for fitting GOME spectra. Determination of the solar reference spectrum has been improved by combining low-resolution information from UARS with high-resolution information as presented in Chance and Spurr, 1997; this is now used in improved wavelength calibration. This information has also now been supplied to the OMI program. Improvements in Ring effect modeling have been made through molecular physics studies employing the best currently available molecular data, development of an improved solar reference spectrum for wavelength-specific applications, and improved determination of the wavelength-dependent Rayleigh scattering cross section [Chance and Spurr, 1997].
- Spectroscopic and aerosol database development, including the production of an improved database of molecular parameters for the visible O₂ A band and improvements to O₃, NO₂, SO₂, BrO, and HCHO reference spectra.
- Participation in the ESA cloud and aerosol *ad hoc* study group to produce cloud and aerosol data products from GOME. Development of the Cloud Retrieval Algorithm for GOME (CRAG/GOMECAT) (mostly with DLR funding).
- Guiding and advising work on operational processor updates and reprocessing of GOME data. This includes, for example, the future use of the TOMS Version 7 ozone climatology in GOME data processing.

- Participating in GOME-2 definition studies, including studies to improve the polarization correction and the undersampling characteristics.

SCIAMACHY

SCIAMACHY is a joint German/Netherlands/Belgian program, with scientific participation from other European countries and, in the U.S., the SAO. SCIAMACHY was successfully launched on Envisat March 1, 2002. SCIAMACHY is currently working nominally and has no major problems except for the buildup of ice on the longest-wave, cooled, infrared detectors, which is currently being addressed by systematic instrument warming procedures. Some initial SCIAMACHY validation has been performed, but no operational products are yet available. It is currently envisaged that Level 1 products will be released during the summer of 2003, and that operational Level 2 products will follow later in 2003 and afterward. SAO continues to participate actively in algorithm development for the level 0-1b and 1b-2 data processing segments, and in SCIAMACHY and other Envisat validation studies.

The SCIAMACHY Science Advisory Group (SSAG) includes K. Chance of the SAO as a U.S. member and head of the Subcommittee for Algorithm Development and Data Usage. J. Geary of the SAO as a U.S. member and advisor on instrument and detector issues, and R. Spurr of the SAO as a U.S. member and organizer and chair of the GOME/SCIAMACHY Scientific Working Sessions. SAO SCIAMACHY studies include the following items:

- Synthetic retrieval studies for atmospheric spectroscopy in the infrared to assess revised estimates of SCIAMACHY detector sensitivity.
- Finalization of the SCIAMACHY band definitions and detector selection criteria; synthetic retrieval studies for atmospheric spectroscopy in the infrared contributing to these definitions.
- Chairing the scientific working subgroup for Algorithm Development and Data Usage; Organizing and chairing the joint GOME/SCIAMACHY Scientific Working Sessions.
- Heading the development, compilation, and production of the Scientific Requirements Document for SCIAMACHY Data and Algorithm Development.
- Radiative transfer studies, including development of line-by-line modeling capability for the infrared and visible and ray tracing for the limb and occultation measurement geometries. The issue of properly combining limb and nadir measurements was addressed in conjunction with the development of the SCIAMACHY observational strategy and in the context of the Algorithm Development and Data Usage subgroup (includes DLR funding).
- Development of LIDORT (see GOME, above).

- Development of the Basic Infrared Absorption Spectroscopy (BIAS) technique for application to the SCIAMACHY infrared channels (includes DLR funding).
- Extension of GOME software development to SCIAMACHY. Existing GOME databases are extended in wavelength where appropriate to the near infrared. New line spectroscopic data sets were compiled for SCIAMACHY channels 7 and 8 (includes DLR funding).
- Participation in the definition of NRT and OL data products for SCIAMACHY, including close collaboration with the DLR in the generation of SCIAMACHY NRT specification documentation. Production and development of the SCIAMACHY Algorithm Theoretical Basis Document. Collaborate with DLR on the development of NRT SCIAMACHY Data Processors, including the provision of test data sets and upgrades to the algorithm descriptions required by industry (includes DLR funding).
- The development of software for the off-line level 1b to 2 processing segment for SCIAMACHY limb measurements has been a major focus at SAO. To this end, a single scatter ray tracing forward model was written for the O₃ limb profile application, and combined with optimal estimation software to produce an end-to-end algorithm. Work continues on limb retrieval from infrared observations, including improved microwindow selection versus tangent height (includes DLR funding).
- Participation in the validation planning for SCIAMACHY, and in initial validation of SCIAMACHY nadir and limb UV/visible data. This includes:
 - Determination of wavelength calibration for SCIAMACHY measurements using the method of *Caspar and Chance* [1997], developed for GOME. Wavelength shifts during limb-scan measurements are substantial, and probably reflect changes in the way the detector arrays are filled during the limb scan. This will need to be addressed in later operational algorithm improvements.
 - Limb-pointing studies to determine pointing from the data themselves rather than deriving it from the onboard star-tracker. This will be necessary to implement in future algorithm versions. We have produced determinations of the limb pointing using complete radiative transfer modeling of the limb spectrum from 290-305 nm. Wavelengths shorter than 305 nm exhibit “knees” in the limb-scattered radiation profile versus altitude which are well determined from radiative transfer modeling for situations where the ozone concentration is under photochemical control (the knee at 305 nm is nominally at 42+ km, depending on solar zenith angle and satellite viewing angle; knees at shorter wavelengths are higher in the atmosphere). We have produced a “multi-knee” method which retrieves the pointing to several hundred meters, but is computationally intensive, and are currently testing a faster method, which has the

advantages of the full radiative-transfer modeled and fitted multi-knee method but which should be sufficiently fast to implement operationally.

- Determination of baseline choices and options for operational processing of SCIAMACHY measurements. This includes the selection criteria and the determination of which options can be pre-tested using GOME data.
- Initial scientific studies on SCIAMACHY nadir and limb data: O_3 , NO_2 , BrO , OCIO , and HCHO .

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